MORSE POTENTIAL AND ITS RELATIONSHIP WITH THE COULOMB IN A POSITION-DEPENDENT MASS BACKGROUND

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Abstract

We provide some explicit examples wherein the Schrödinger equation for the Morse potential remains exactly solvable in a position-dependent mass background. Furthermore, we show how in such a context, the map from the full line $(-\infty, \infty)$ to the half line $(0, \infty)$ may convert an exactly solvable Morse potential into an exactly solvable Coulomb one. This generalizes a well-known property of constant-mass problems.

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Morse potential plays an important physical role in quantum mechanics (see, e.g., [1]). It is an exactly solvable potential and is of much use in spectroscopic applications. It is also known to have a connection with the Coulomb potential under a coordinate transformation — a feature well exploited [2, 3] to describe supersymmetry for the hydrogen atom.

In this note we report on certain characteristics of a one-dimensional Morse potential in a position-dependent mass (PDM) background. There has been considerable interest in PDM problems for some time [4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28]. Indeed there exists a wide variety of situations in which PDM is of utmost relevance [29]. PDM also holds out to deformations in the quantum canonical commutation relations or curvature of the underlying space [30]. Furthermore, it has recently been observed that there exists a whole class of Hermitian PDM Hamiltonians which, to lowest order of perturbation theory, have a correspondence with pseudo-Hermitian Hamiltonians [31].

In a series of papers [20, 21, 22, 23], we extensively discussed the solutions of the one-dimensional Schrödinger equation with PDM in the kinetic energy operator. We explored, in particular, its matching with the coordinate-transformed constant-mass version and the consequent decoupling of the ambiguity parameters appearing in the effective potential. We also looked into the viable choices of the mass function (see also [9, 10]).

Here we show that an exponential choice for the PDM allows one to transform the corresponding Morse Hamiltonian into the constant-mass problem. The eigenfunctions of the latter being known, it is a simple exercise to determine those of the former. On the other hand, a mapping to the half line $(0, \infty)$ results in the expected conversion of the full line $(-\infty, \infty)$ Morse into the Coulomb. We then demonstrate how to identify the Coulomb potential in the presence of PDM. We also provide estimates of the potential parameter, modified angular momentum quantum number and energy eigenvalues in such a setting.

The one-dimensional effective PDM Hamiltonian is given by [32]

$$H_{\text{eff}} = -\frac{d}{dx} \frac{1}{M(x)} \frac{d}{dx} + V_{\text{eff}}(x), \tag{1}$$

where $V_{\text{eff}}(x)$ contains the given potential $V(x)$:

$$V_{\text{eff}}(x) = V(x) + \frac{1}{2}(\beta+1)\frac{M''}{M^2} - [\alpha(\alpha+\beta+1)+\beta+1]\frac{M'^2}{M^3}. \tag{2}$$

In (2), α, β are the ambiguity parameters and primes stand for the derivatives with respect to x. We use the dimensionless form $M(x)$ of the mass function $m(x) = m_0 M(x)$ and adopt units such that $\hbar = 2m_0 = 1$.

The Schrödinger equation corresponding to (1) is

$$\left(-\frac{1}{M}\frac{d^2}{dx^2} + \frac{M'}{M^2}\frac{d}{dx} + V_{\text{eff}} - \epsilon\right)\varphi(x) = 0, \tag{3}$$

where the first-derivative term can be removed by the transformation $\varphi = \sqrt{M}\,\psi$:

$$\left(-\frac{1}{M}\frac{d^2}{dx^2} + \frac{3}{4}\frac{M'^2}{M^3} - \frac{1}{2}\frac{M''}{M^2} + V_{\text{eff}} - \epsilon\right)\psi(x) = 0. \tag{4}$$

Let us set for $M(x)$ and $V(x)$ the following forms

$$M(x) = e^{-2x}, \qquad V(x) = V_0 e^{2x} - B(2A+1)e^{x}, \tag{5}$$

where V_0, A and B are coupling parameters. It then follows from (4) that

$$\left\{-\frac{d^2}{dx^2} + U(x) + V_0 - [4\alpha(\alpha+\beta+1) + 2(\beta+1) - 1]\right\}\psi(x) = 0, \tag{6}$$

where $U(x) = B^2 e^{-2x} - B(2A+1)e^{-x}$ and we have put $\epsilon = -B^2$ for notational reasons. We thus find that the Morse potential $V(x)$ with an exponential PDM can be transformed into the standard $U(x)$ with constant mass.[a] With $V_0 = (A-n)^2 + [4\alpha(\alpha+\beta+1) + 2\beta + 1]$, the energy eigenvalues of the latter can be cast as [34]

$$E_n = -(A-n)^2, \qquad n = 0, 1, \ldots, n_{\max}\ (n_{\max} < A). \tag{7}$$

Further, the corresponding wavefunctions can be expressed as

$$\psi_n(x) \propto y^{A-n} e^{-\frac{1}{2}y} L_n^{(2A-2n)}(y), \qquad y = 2Be^{-x}. \tag{8}$$

[a] Actually, for some appropriate choices of parameters, $U(x)$ coincides with the potential proposed by Morse [33], while $V(x)$ is an alternative (often used) form obtained by applying the parity transformation $x \to -x$.

It is now straightforward to derive the wavefunctions of (3) by employing the relation $\varphi = e^{-x}\psi$. We obtain

$$\varphi_n(x) \propto y^{A+1-n} e^{-\frac{1}{2}y} L_n^{(2A-2n)}(y). \tag{9}$$

One can see $\varphi_n(x)$ to be square integrable on $(-\infty, \infty)$. Moreover for $x \to \infty$, the condition $|\varphi_n(x)|^2/\sqrt{M(x)} \sim e^{-(2A+1-2n)x} \to 0$ is fulfilled which, as has been established elsewhere [22], is appropriate for a vanishing mass at $x \to \infty$.

It must be stressed that other choices of mass functions can be made which work well for the Morse potential. It is also interesting to observe that the following form for $M(x)$,

$$M(x) = \frac{1}{(1 + \kappa e^x)^2} \qquad (\kappa > 0), \tag{10}$$

renders both $V(x)$ and $V_{\text{eff}}(x)$ Morse-like. Indeed plugging in $V(x)$ from (5) (where we have reset $V_0 = B^2$) gives

$$V_{\text{eff}}(x) = B'^2 e^{2x} - B'(2A' + 1)e^x, \tag{11}$$

where $B'^2 = B^2 - 2[2\alpha(\alpha+\beta+1)+\beta+1]\kappa^2$ and $B'(2A'+1) = B(2A+1)+(\beta+1)\kappa$. Notice that like $V(x)$, $V_{\text{eff}}(x)$ is also Morse but has the coefficients scaled. In terms of the new parameters A', B', the energy eigenvalues turn out to be

$$\epsilon_n = -\frac{1}{4}\left(\frac{2B'(2A'+1) - [(2n+1)\Delta + 2(n^2+n+1)\kappa]}{\Delta + (2n+1)\kappa}\right)^2 \tag{12}$$

in which $\Delta = 2\sqrt{B'^2 + \kappa^2}$. The corresponding wavefunctions $\varphi_n(x)$ can also be determined. For the ground state, for instance, one finds the function

$$\begin{aligned} \varphi_0(x) &\propto (1 + \kappa e^x)^{\frac{\lambda}{\kappa} - \mu - \frac{1}{2}} e^{\mu x}, \\ \lambda &= -\frac{1}{2}(\Delta + \kappa), \qquad \mu = \frac{1}{2}\left(\frac{2B'(2A'+1) - \kappa}{\Delta + \kappa} - 1\right), \end{aligned} \tag{13}$$

which is square integrable on $(-\infty, \infty)$ and satisfies the condition $|\varphi_0(x)|^2/\sqrt{M(x)} \to 0$ for $x \to \infty$, as it should be.

We now turn to the Coulomb problem.

A coordinate transformation $x = \ln r$ transforms a full line $(-\infty, \infty)$ to a half line $(0, \infty)$. Making this change of variable, Eq. (3) gets modified to the form

$$\left[-\frac{1}{\bar{M}} \frac{d^2}{dr^2} + \frac{1}{\bar{M}} \left(\frac{\dot{\bar{M}}}{\bar{M}} - \frac{1}{r} \right) \frac{d}{dr} + \frac{1}{r^2} \left(\hat{V}_{\text{eff}} - \epsilon_n \right) \right] \bar{\varphi}_n(r) = 0, \tag{14}$$

where we have denoted

$$\begin{aligned} \bar{M}(r) &= M(x(r)) = \frac{1}{(1+\kappa r)^2}, \qquad \bar{\varphi}_n(r) = \varphi_n(x(r)), \\ \hat{V}_{\text{eff}}(r) &= V_{\text{eff}}(x(r)) = B'^2 r^2 - B'(2A'+1) r, \end{aligned} \tag{15}$$

and indicated by an overhead dot a derivative with respect to r.

A further substitution $\bar{\varphi}(r) = \sqrt{r}\, \chi(r)$ results in the three-dimensional form of the PDM radial Schrödinger equation

$$\left[-\frac{1}{\bar{M}} \frac{d^2}{dr^2} + \frac{1}{\bar{M}} \left(\frac{\dot{\bar{M}}}{\bar{M}} - \frac{2}{r} \right) \frac{d}{dr} + \frac{l(l+1)}{\bar{M} r^2} + \bar{V}_{\text{eff}} - E \right] \chi_{nl}(r) = 0, \tag{16}$$

in which l is the angular momentum quantum number and $\bar{V}_{\text{eff}}(r)$ is given by

$$\bar{V}_{\text{eff}}(r) = -\frac{1}{\bar{M}} \left(-\frac{1}{2r} \frac{\dot{\bar{M}}}{\bar{M}} + \frac{\left(l + \frac{1}{2}\right)^2}{r^2} \right) + \frac{1}{r^2} \left(\hat{V}_{\text{eff}} - \epsilon_n \right) + E. \tag{17}$$

Note that Eq. (16) could also be arrived at if we generalized (1) to three dimensions [28] and carried out the usual separation of variables in the corresponding Schrödinger equation.

Actually we can convert (16) to the typical one-dimensional form (1), namely

$$\left(-\frac{d}{dr} \frac{1}{\bar{M}} \frac{d}{dr} + \tilde{V}_{\text{eff}} - E \right) \xi_{nl}(r) = 0, \tag{18}$$

if we set $\chi(r) = \frac{1}{r} \xi(r)$ and define $\tilde{V}_{\text{eff}}(r)$ as

$$\tilde{V}_{\text{eff}}(r) = \bar{V}_{\text{eff}} - \frac{\dot{\bar{M}}}{\bar{M}^2 r} + \frac{l(l+1)}{\bar{M} r^2}. \tag{19}$$

For the choice of mass function in (15), $\tilde{V}_{\text{eff}}(r)$ becomes

$$\tilde{V}_{\text{eff}}(r) = -\frac{B'(2A'+1) + \frac{\kappa}{2}}{r} - \frac{\epsilon_n + \frac{1}{4}}{r^2} + E + B'^2 + \frac{3}{4}\kappa^2. \tag{20}$$

We conclude that the function $\xi_{nl}(r)$ satisfies the equation

$$\left(-\frac{d}{dr}\frac{1}{\bar{M}}\frac{d}{dr}-\frac{2Z}{r}+\frac{l(l+1)}{r^2}-\frac{1}{4}\kappa^2-\lambda_{nl}\right)\xi_{nl}(r)=0 \tag{21}$$

and may be interpreted to be the one satisfied by the Coulomb potential $-\frac{2Z}{r}$ in the presence of PDM. In (21), we defined

$$2Z=B'(2A'+1)-\frac{\kappa}{2}, \qquad l(l+1)=-\epsilon_n-\frac{1}{4}, \qquad \lambda_{nl}=-B'^2-\kappa^2. \tag{22}$$

In the constant-mass case ($\kappa=0$), we have $A'=A$, $B'=B$, $\epsilon_n=-(A-n)^2$. On using (22), we get

$$Z=B\left(A+\frac{1}{2}\right), \qquad l=A-n-\frac{1}{2}, \qquad \lambda_{nl}=-\frac{Z^2}{(n+l+1)^2}, \tag{23}$$

and so Eq. (21) coincides with the standard radial equation of the Coulomb potential, where λ_{nl} denotes the energy eigenvalues.

Finally, from (22) we can obtain solutions for Z, l and the eigenvalues λ_{nl} as follows:

$$\begin{aligned} Z &= B'\left(A'+\frac{1}{2}\right)-\frac{\kappa}{4}, \\ l &= \frac{2B'(2A'+1)-[2(n+1)\Delta+(2n^2+4n+3)\kappa]}{2[\Delta+(2n+1)\kappa]}, \\ \lambda_{nl} &= -\left(\frac{2Z-[n^2+(l+1)(2n+1)]\kappa}{2(n+l+1)}\right)^2, \end{aligned} \tag{24}$$

where we have used ϵ_n given by (12). These are to be interpreted as modified expressions of the parameter Z, the angular momentum quantum number and the eigenvalues in the presence of PDM.

The corresponding wavefunctions can be easily found from the relation $\xi_{nl}(r)=\sqrt{r}\,\bar{\varphi}_n(r)$. From (13), for instance, we get

$$\xi_{0l}(r)\propto r^{\mu+\frac{1}{2}}(1+\kappa r)^{\frac{\lambda}{\kappa}-\mu-\frac{1}{2}}, \tag{25}$$

which can be rewritten as

$$\xi_{0l}(r)\propto r^{l+1}(1+\kappa r)^{-\left(\frac{Z}{(l+1)\kappa}+l+1\right)} \tag{26}$$

as a consequence of (13), (22) and (24). It can be easily checked that such a transformed wavefunction is square integrable on $(0, \infty)$ and fulfils the condition $|\xi_{0l}(r)|^2/\sqrt{\bar{M}(r)} \to 0$ for $r \to \infty$.

As a final comment, it is worth observing that nonnegative integer values of l in (24)[b] are associated with some specific choices for the Morse potential and mass parameters A', B', κ. This, however, is by no way a new feature due to the PDM environment since it can be seen from (23) that a similar restriction exists for A and B in the constant-mass case.

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[b]The requirement of integer Z values may be relaxed since in atomic physics an effective parameter Z_{eff} is often used [1].

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